Assessment of nuclear data libraries for SFR simulation using SCALE Code System

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2023 SCALE Users' Group Workshop
26-28 November 2023
Oak Ridge National Laboratory (hybrid meeting)

Motivation

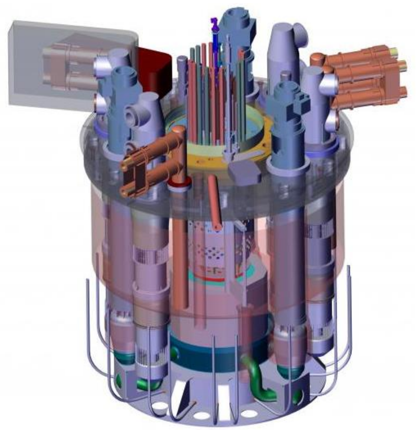
- Increasing interest in liquid metal fast reactors (LMFR)
- In recent years, UPM has participated into different European R&D projects
- … with a common objective: validate computational approaches to support the development of LMFR
- This involves the verification and validation (V&V) of computational tools and associated databases.
- Our activities rely on the use of **SCALE Code System**

ESNII+

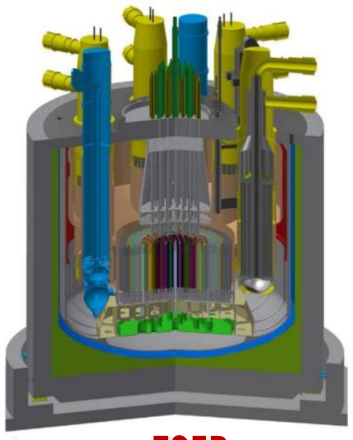
CHANDA
SOLVING CHALLENGES IN NUCLEAR DATA FOR THE SAFETY OF EUROPEAN NUCLEAR FACILITIES

ESFR-SMART
sodium fast reactor safety

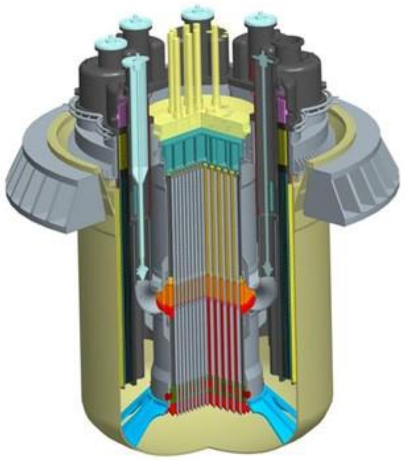
SANDA
Supplying Accurate Nuclear Data for energy and non-energy Applications
HORIZON2020



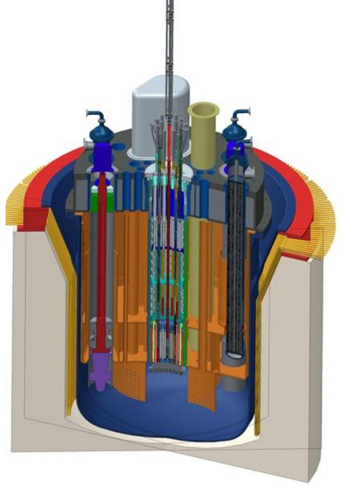
ASTRID
(1500 MWth)



ESFR
(3600 MWth)



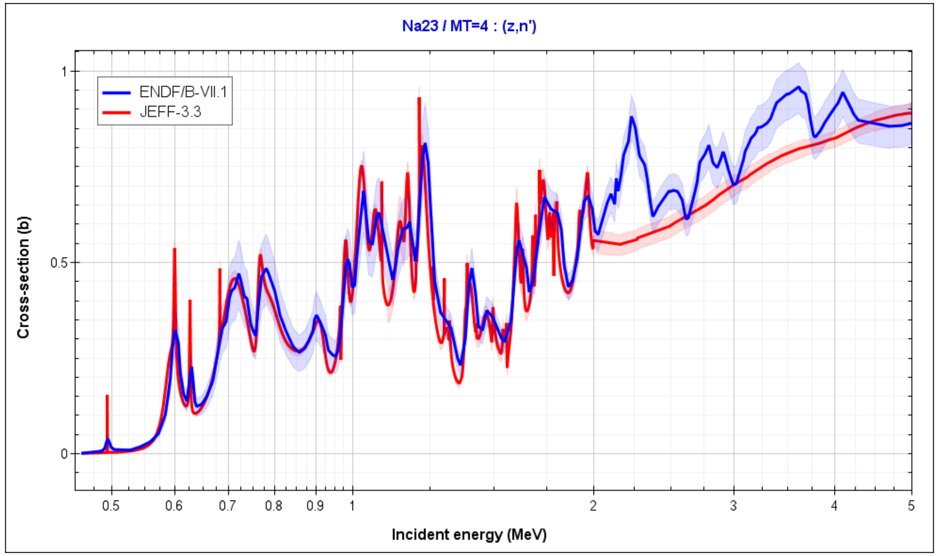
LFR ALFRED
(300 MWth)



LFR MYRRHA
(100 MWth)

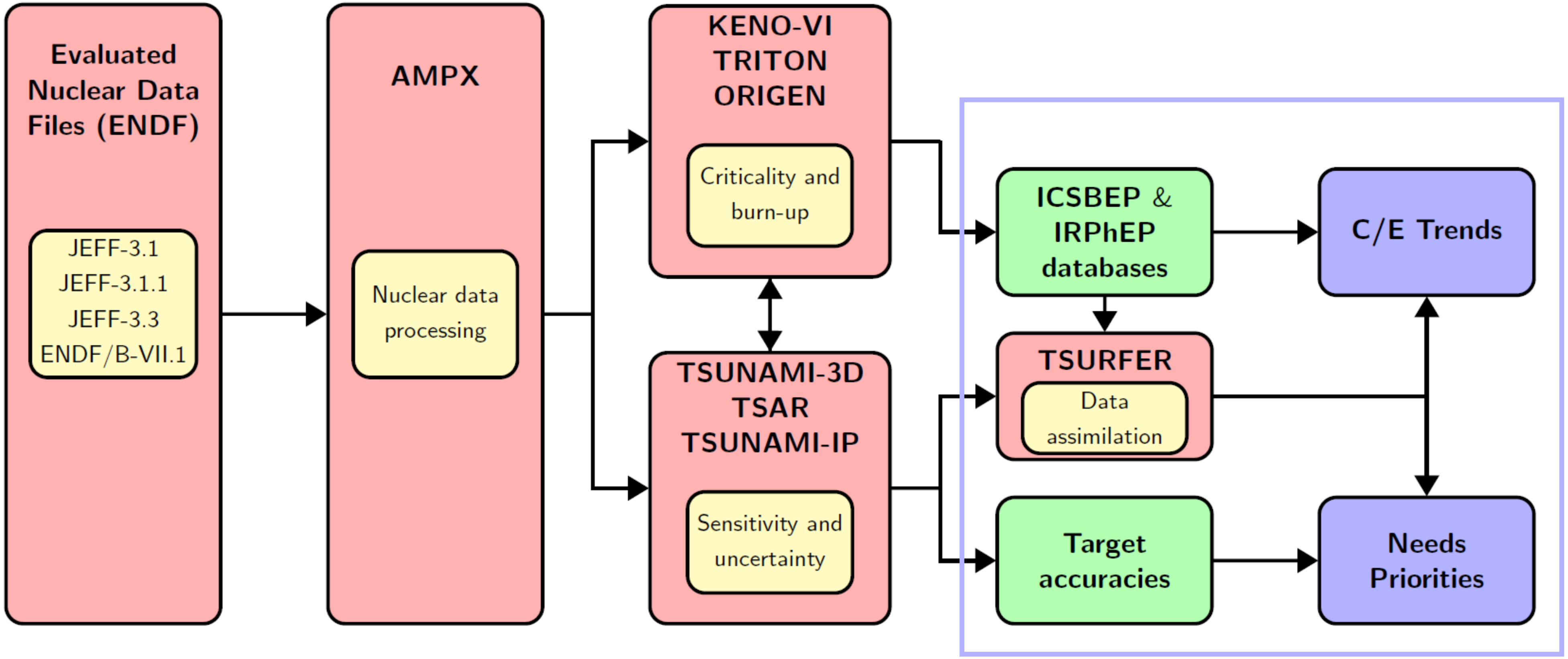
Motivation

- **Nuclear data libraries**, as part of the computational scheme, are subject to V&V
- A reasonable level of knowledge has still not been reached for all the isotopes and reactions involved in spite of several decades of research
- The use of different nuclear data libraries may lead to very different results, with a different uncertainty quantification.
- Then, V&V activities carried out in our work aim at evaluating the performance of the JEFF-3.3 library for SFR simulation.
- Systematic use of legacy integral experiments provided by ICSBEP and IRPhEP databases.



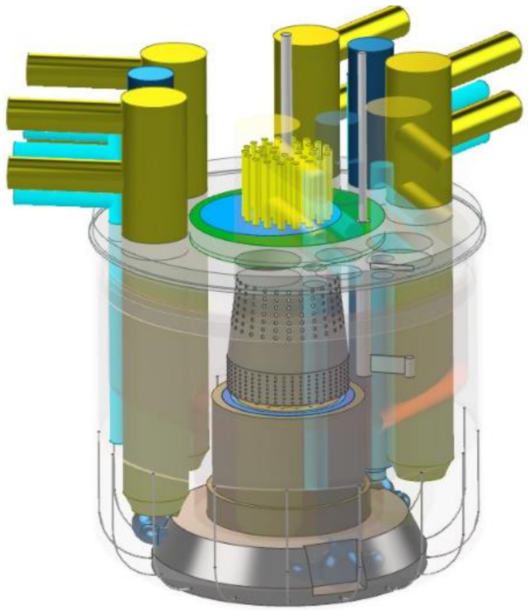
Na-23 (n,n') cross section from JEFF-3.3 and ENDF/B-VII.1

Nuclear data assessment: pipeline

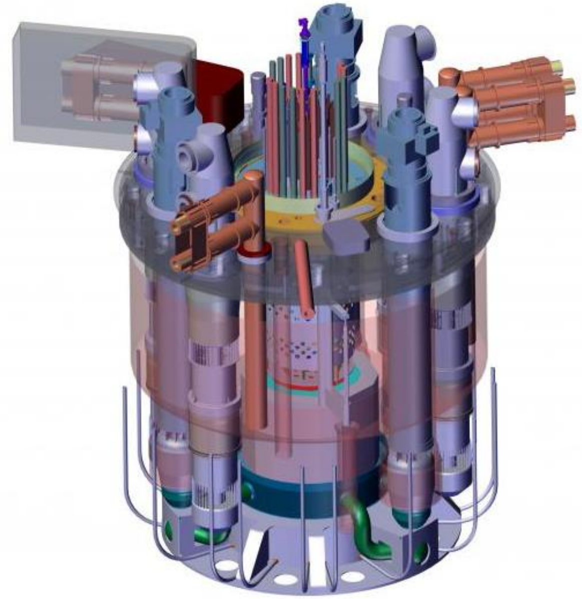


A. Jiménez-Carrascosa, N. García-Herranz. *"Use of SCALE for the analysis of Sodium Fast Reactors,"* **SCALE Users' Group Workshop 2021.**

SFR systems under analysis



ESFR
European **S**odium **F**ast **R**eactor
(Commercial-size 3600 MWth core)[1]



ASTRID-like
Advanced **S**odium **T**echnological **R**eactor for **I**ndustrial **D**emonstration
(Medium-size 1500 MWth core)[2]

(1) A. Rineiski et al., H2020 ESFR-SMART Project, D1.1.2, for the heterogeneous core (ESFR)
(2) P. Sciora, FP7 ESNII+ Project, deliverable D6.1.1-1 (ASTRID)

Computational tools and nuclear data

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SCALE 6.2.3 Code System

Advanced reactor evaluation

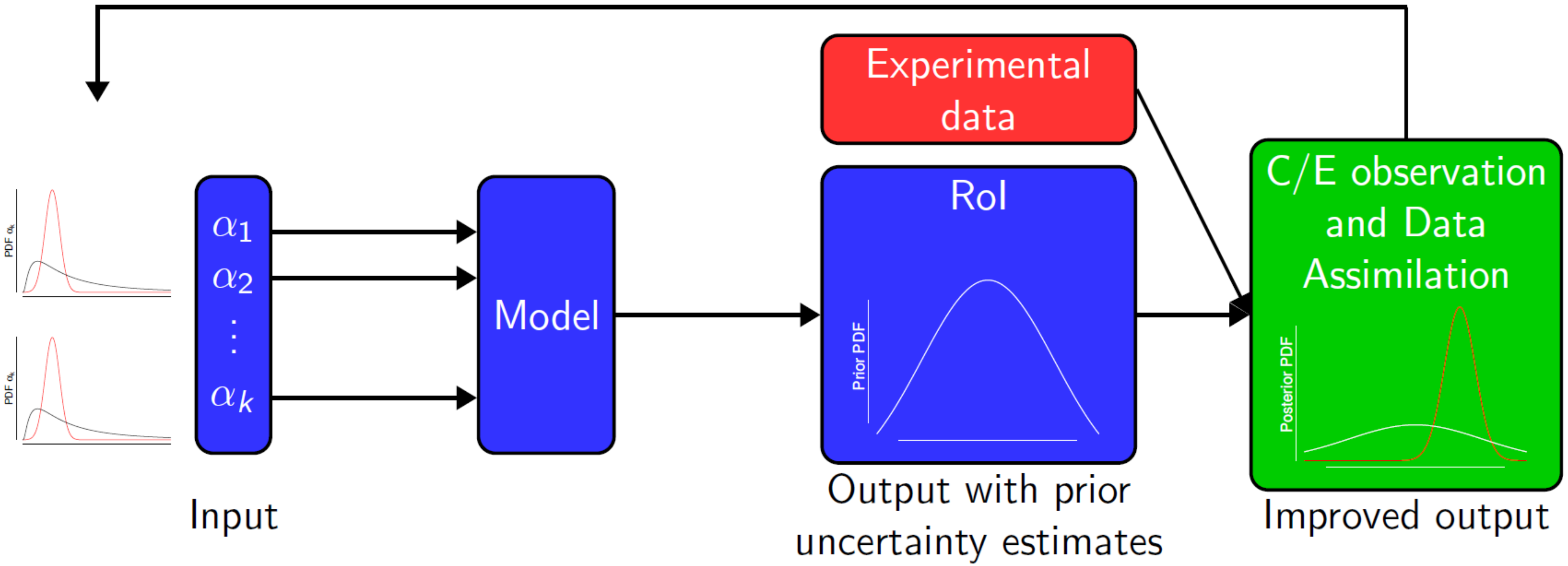
- Criticality calculations using **KENO-VI**
- **CE JEFF-3.3 and CE ENDF/B-VII.1**
- Sensitivities using **TSUNAMI-3D and TSAR**
- Uncertainties via the Sandwich Rule and **33g JEFF-3.3 covariance matrix** (COVERX-formatted)

Integral experiments evaluation

- Criticality calculations using **KENO-VI**
- **CE JEFF-3.3, CE ENDF/B-VII.1 and/or CE JEFF-3.1.1**
- **Two different sets of experiments,**
  - ICSBEP criticality experiment benchmarks
  - IRPhEP reactor physics experiment benchmarks with reactivity effects

Computational tools and nuclear data

Framework of Data Assimilation: GLLS-based TSURFER module



Information provided by experimental data is transferred to the employed nuclear data library, JEFF-3.3, to improve the model output with constraint uncertainties.

Results for advanced SFR

- Impact of different nuclear data libraries on SFR parameters:

Reactor	Response	Nominal value JEFF-3.3	Nominal value ENDF/B-VII.1	Difference (pcm)	Uncertainty [%] JEFF-3.3 COV	Target accuracy (OECD/NEA WPEC SG46)
ESFR	Multiplication factor k_{eff}	1.00378	1.00072	306	1.03	0.3%
	Sodium void effect ρ_{Na}	500	270	230	15.7	5%
	Doppler effect ρ_T	-134	-121	-13	4.4	5%
ASTRID	Multiplication factor k_{eff}	1.00296	0.99936	360	0.97	0.3%
	Sodium void effect ρ_{Na}	-375	-581	206	22.55	5%

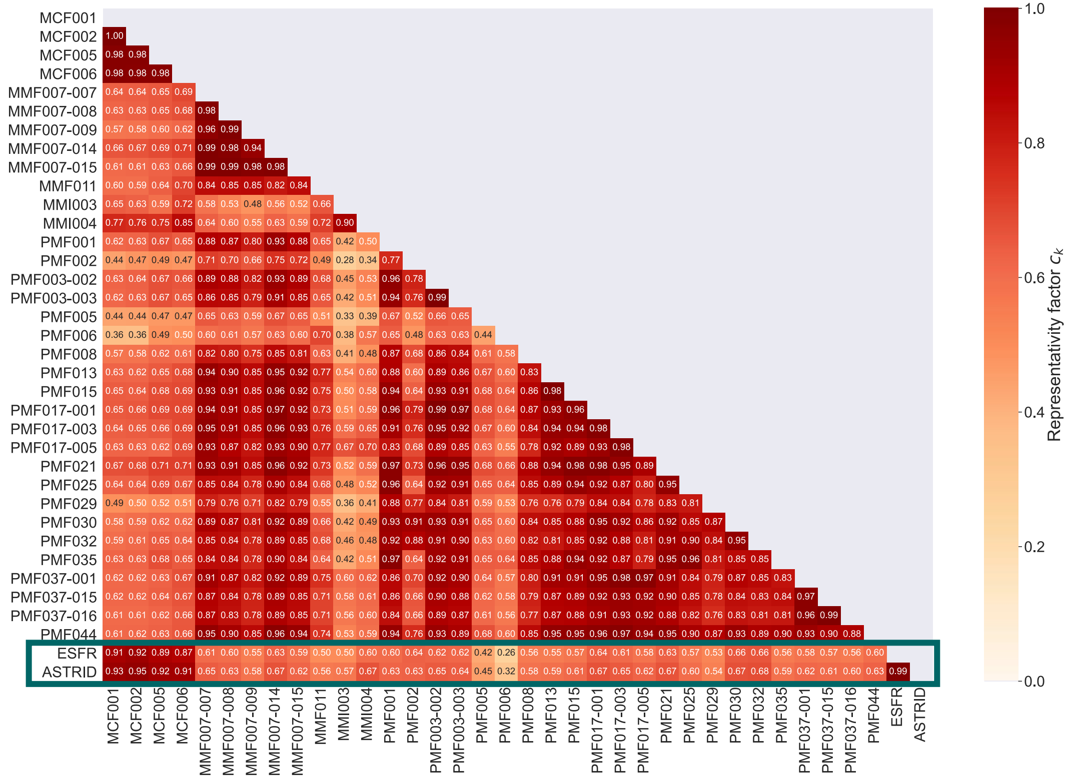
- JEFF-3.3 overestimates both multiplication factor and sodium void worth effect compared to ENDF/B-VII.1.
- Target accuracies exceeded for k_{eff} and ρ_{Na}.

Integral experiments selection (ICSBEP)

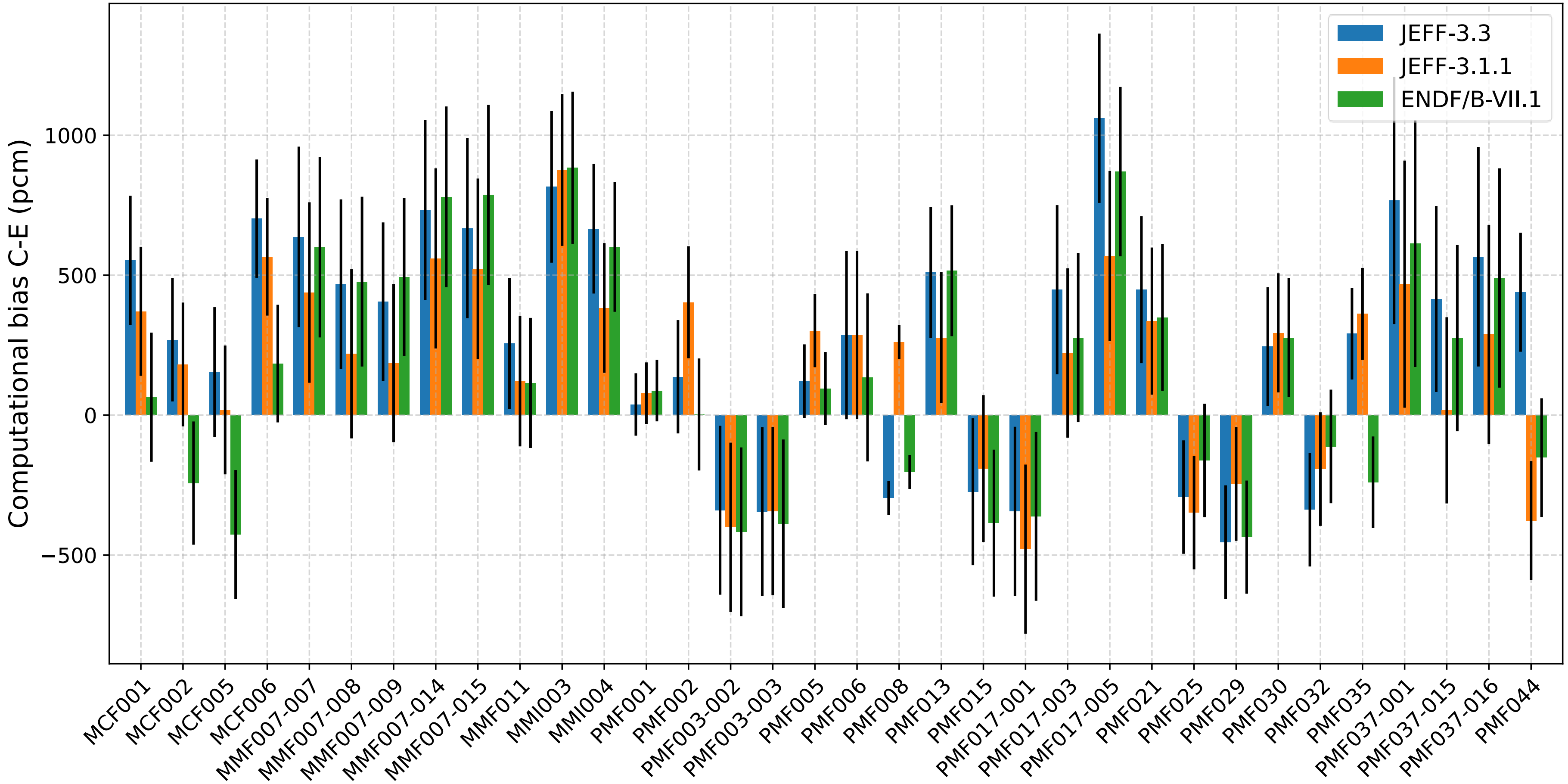
A set of **34 integral experiments benchmarks from ICSBEP** is selected based on the representativity factor with ESFR (TSUNAMI-IP):

$$c_k = \frac{S_{R,\alpha}^T V_{\alpha,\alpha} S_{E,\alpha}}{\sqrt{(S_{R,\alpha}^T V_{\alpha,\alpha} S_{R,\alpha})(S_{E,\alpha}^T V_{\alpha,\alpha} S_{E,\alpha})}}$$

Benchmark experimental series	Evaluators
MIX-COMP-FAST (4 cases)	ANL, USA
MIX-MET-FAST (6 cases)	LLNL and ANL, USA
MIX-MET-INTER (2 cases)	ANL, USA
PU-MET-FAST (22 cases)	LLNL and LANL, USA / IPPE, VNIEEF and CML, Russia

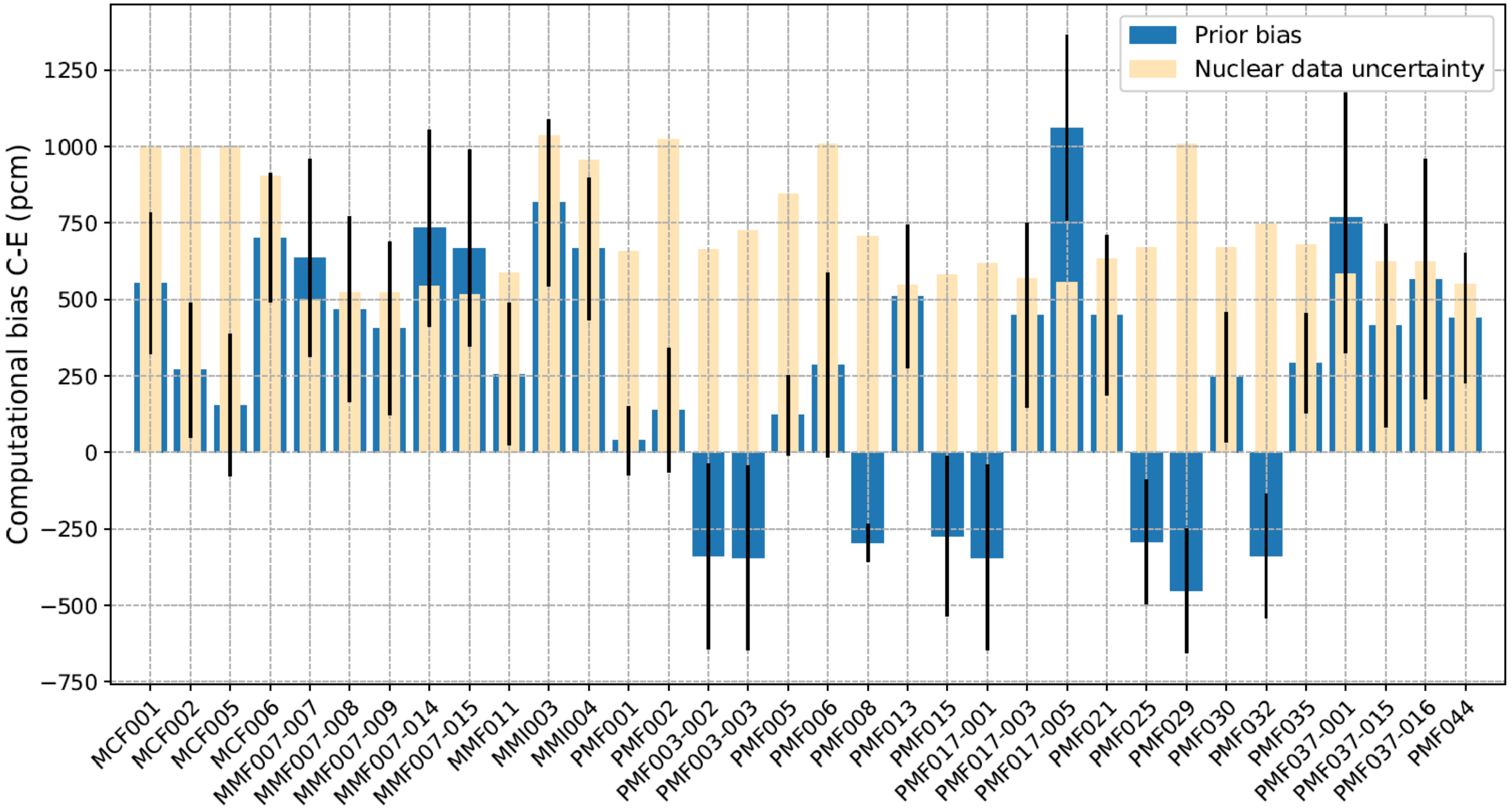


Results for integral experiments (C/E)



- **Average C-E deviation of 440 pcm for JEFF-3.3 results while both JEFF-3.1.1 and ENDF/B-VII.1 perform slightly better (MAD: 329 and 368 pcm, respectively)**
- **Special attention should be paid to MIX-COMP-FAST benchmarks since associated trends will similarly impact on selected SFR systems.**
- **Systematic overestimation for the MIX benchmarks**
- **Additionally, PU-MET-FAST cases ensure a proper adjustment for Pu isotopes.**

Results for integral experiments (C/E)



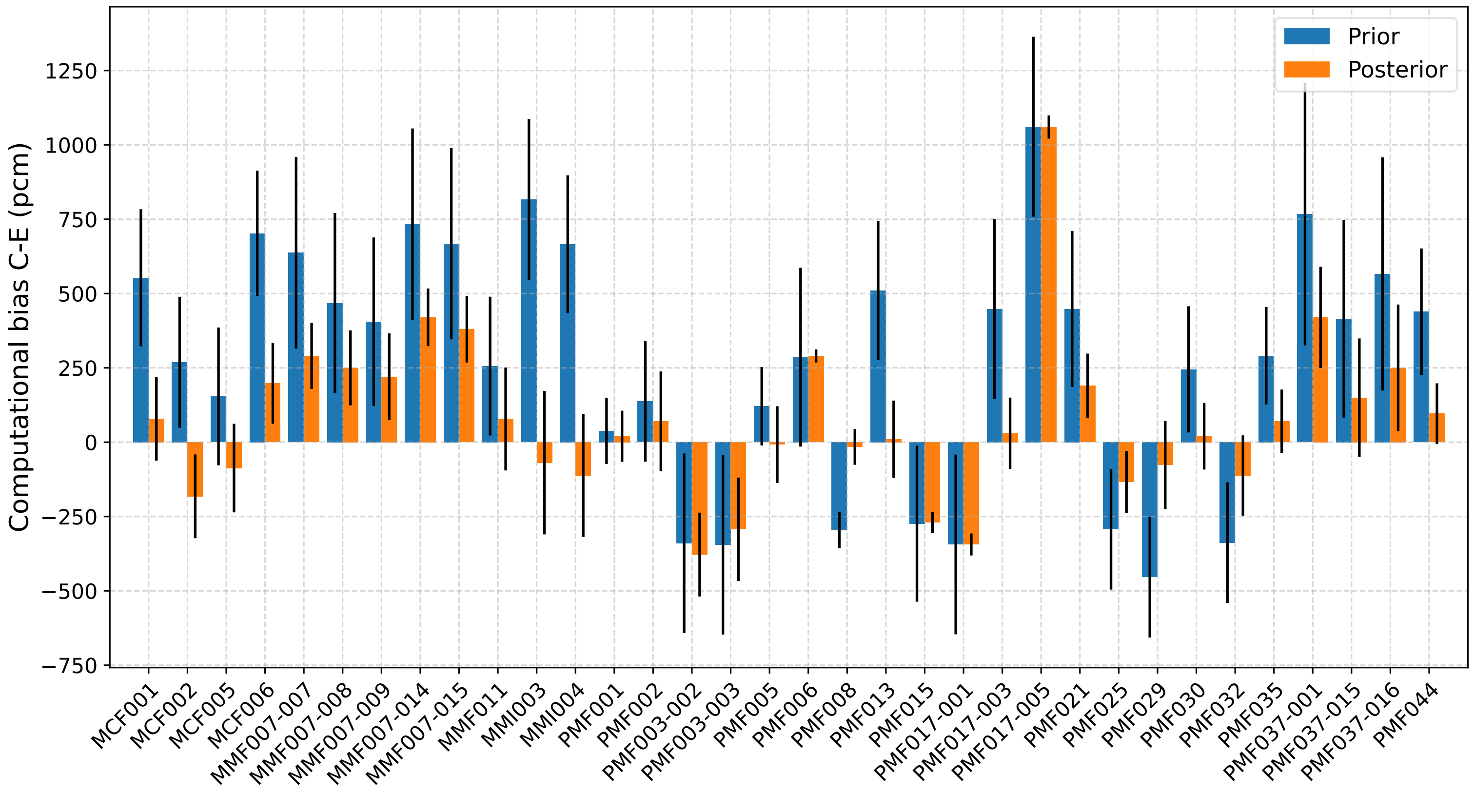
- **Evaluation of nuclear data-induced uncertainty for each case.**
- **Adjustment margin within the 1σ range.**
- **Experiment merit:** are the biases already covered by experimental and computational uncertainties?
- **Role of chi-filtering.**

Data assimilation for ICSBEP data set

- The established experimental database is applied with the aim of improving JEFF-3.3 results.
- Experiments might be ommited through the chi-filtering in TSURFER.
- The following information is required before performing the adjustment:
  - Prior JEFF-3.3 nuclear data covariance matrix,
  - Sensitivity profiles for every experiment response,
  - Active responses: integral experiment benchmarks,
  - Passive responses: target SFR designs under analysis,
  - Experiment covariance data: **scarcely available!** Conservative assumptions to be made.
- As a result, a set of MG adjusted cross section and covariance data set is obtained.

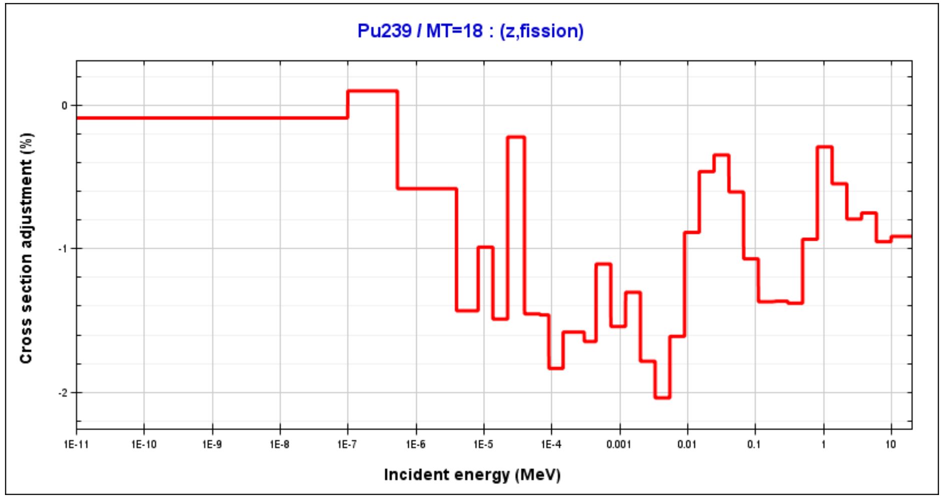
Data assimilation for ICSBEP data set

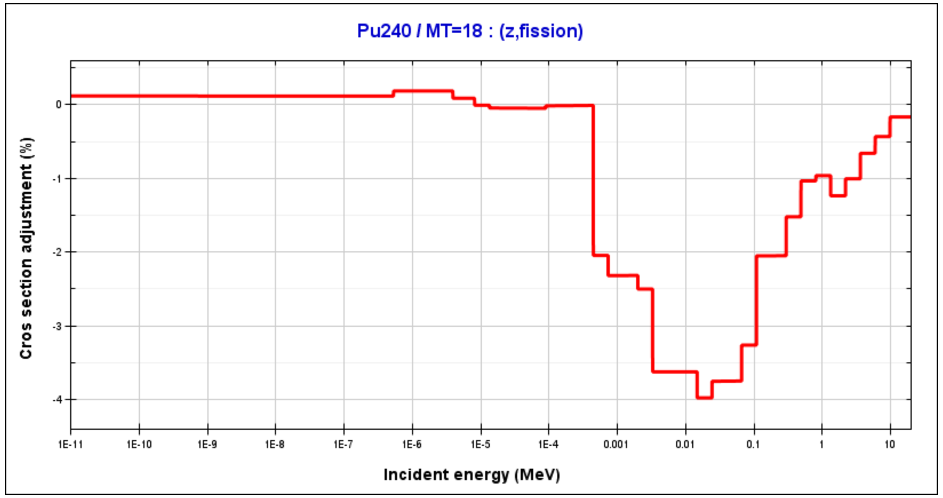
MG cross-section adjustment leads to the following **biases reduction**

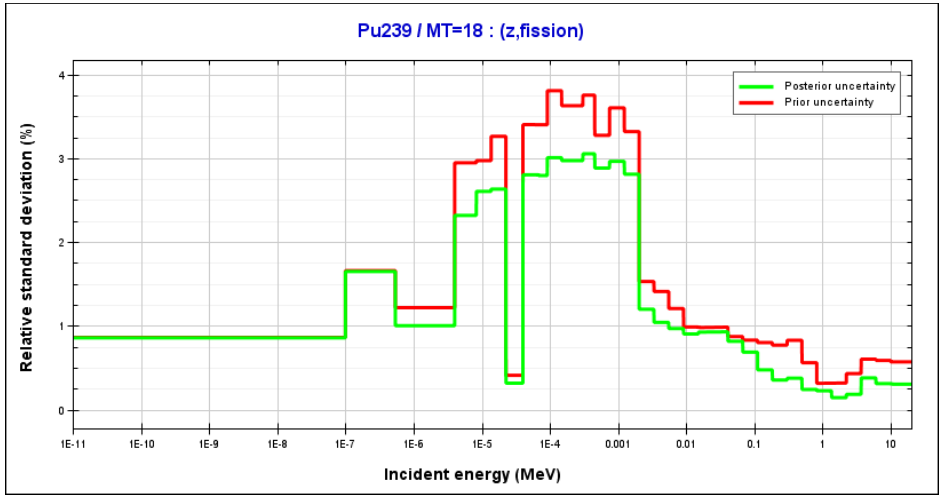


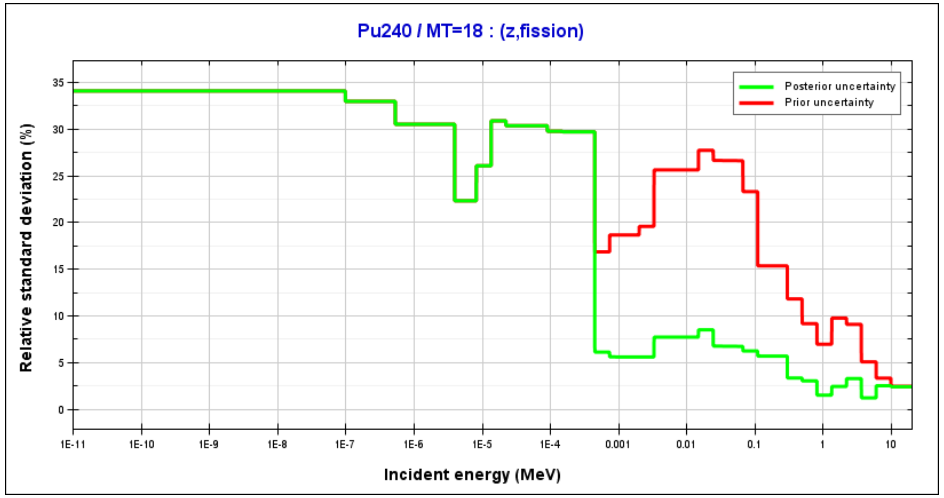
- Mean Absolute Deviation reduces from 440 to 196 pcm
- A systematic reduction of C-E is obtained for MIX benchmarks
- For MIX-COMP-FAST, adjustment provides a more consistent C/E observation
- Major adjustments for the following isotopes:
    - Pu-239 (n,f), χ, (n,γ), nubar
    - U-238 (n,n’), (n,γ), (n,f)
    - Pu-240 (n,f)
    - Fe-56 (n,n’)

Data assimilation for ICSBEP data set









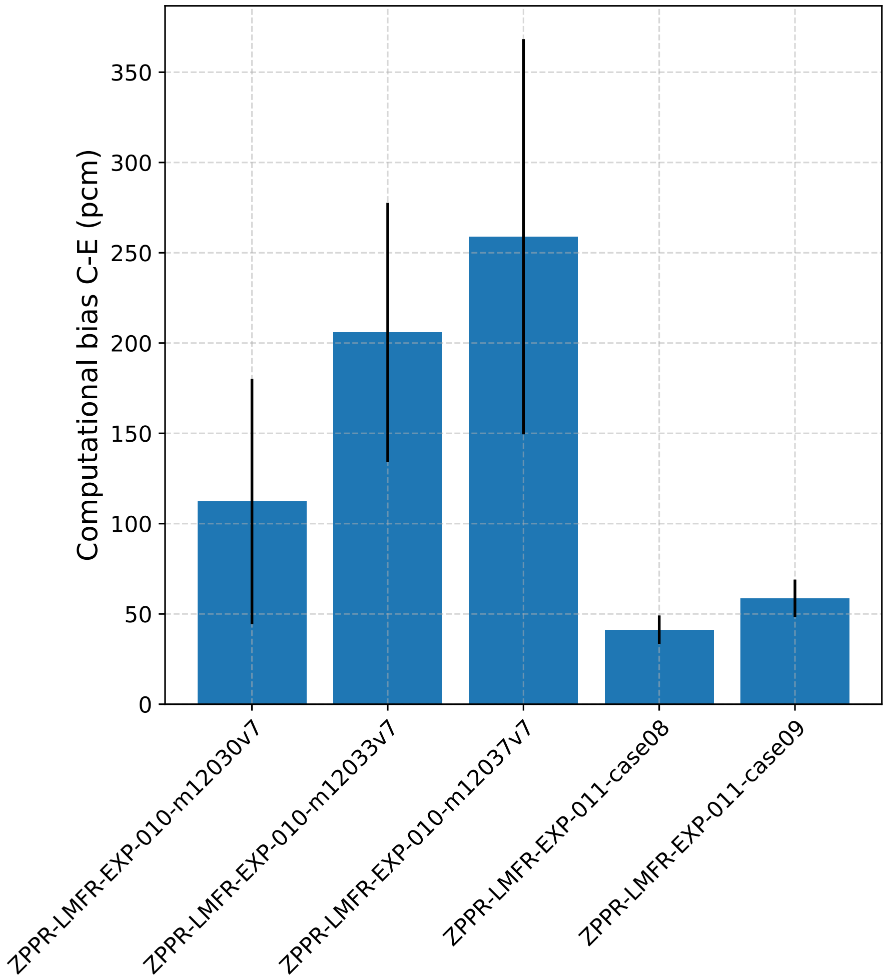
Data assimilation for ICSBEP data set

Impact of data assimilation on SFR designs parameters

Reactor	Response	Prior value	Posterior value	Bias (pcm)	Prior uncertainty (%)	Posterior uncertainty (%)
ESFR	Multiplication factor k_{eff}	1.00378	1.0005	-329	1.036	0.294
	Sodium void effect ρ_{Na}	500	558	+58	15.68	11.11
	Doppler effect ρ_T	-134	-134	0	4.41	2.45
ASTRID	Multiplication factor k_{eff}	1.00296	0.99926	-370	0.970	0.237
	Sodium void effect ρ_{Na}	-375	-300	+75	22.55	14.92

- Significant decrease for multiplication factor values, applying to both designs.
- Strong uncertainty reduction, especially for k_{eff} values fulfilling target accuracies!
- Reinforcement of the sodium void effect. This is not consistent with our extended observations!

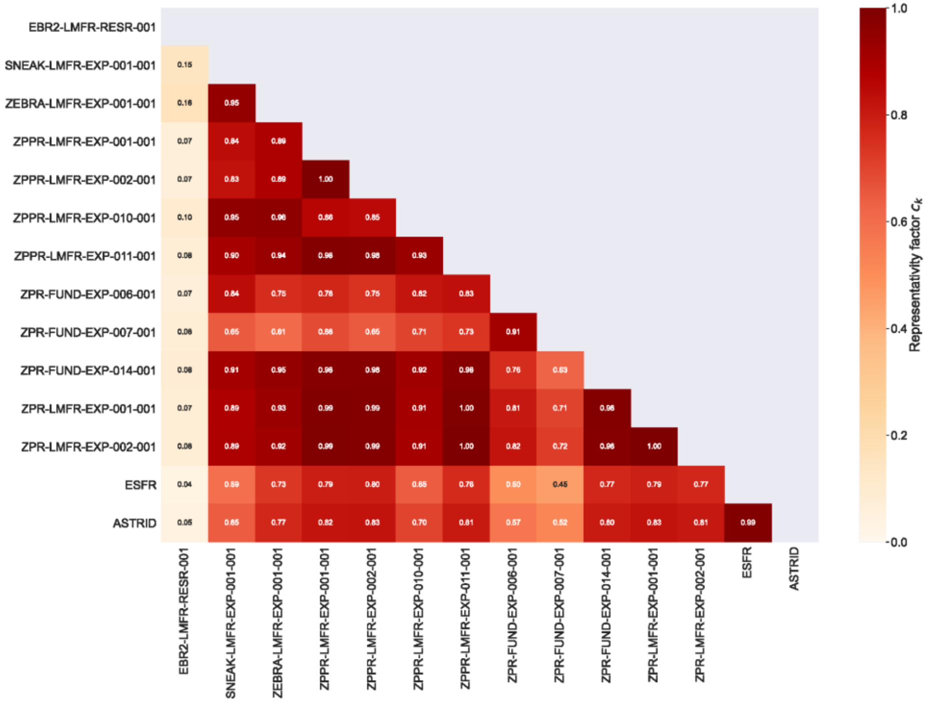
C/E observations for SVR effects

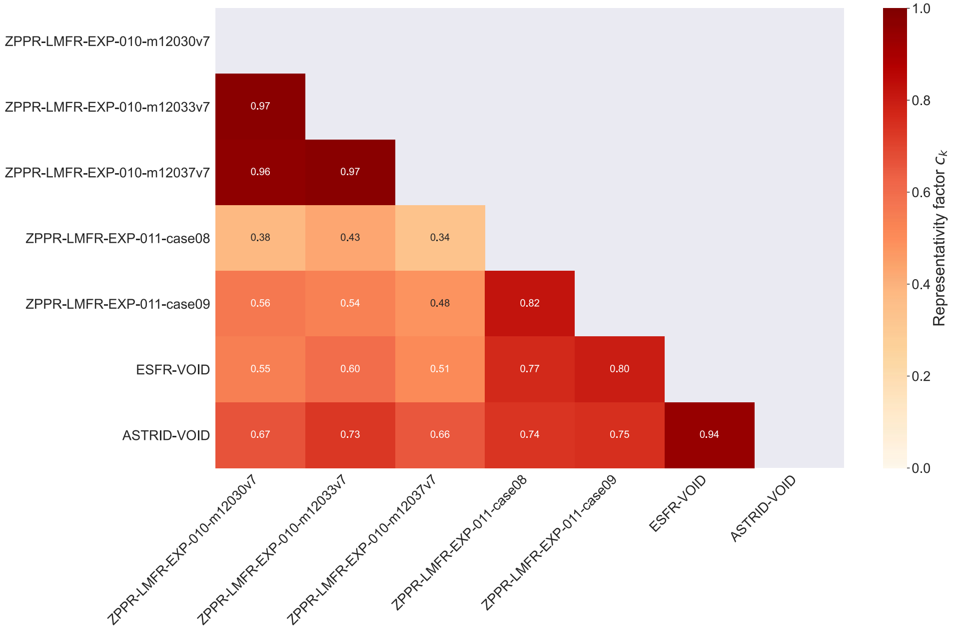


- Significant and systematic overestimation for SVR when using JEFF-3.3
- This trend is observed for several ZPPR experimental measurements (high c_k value compared to ESFR SVR)
- **A complete IRPhEP database should be selected to perform more comprehensive adjustments, involving reactivity effects**

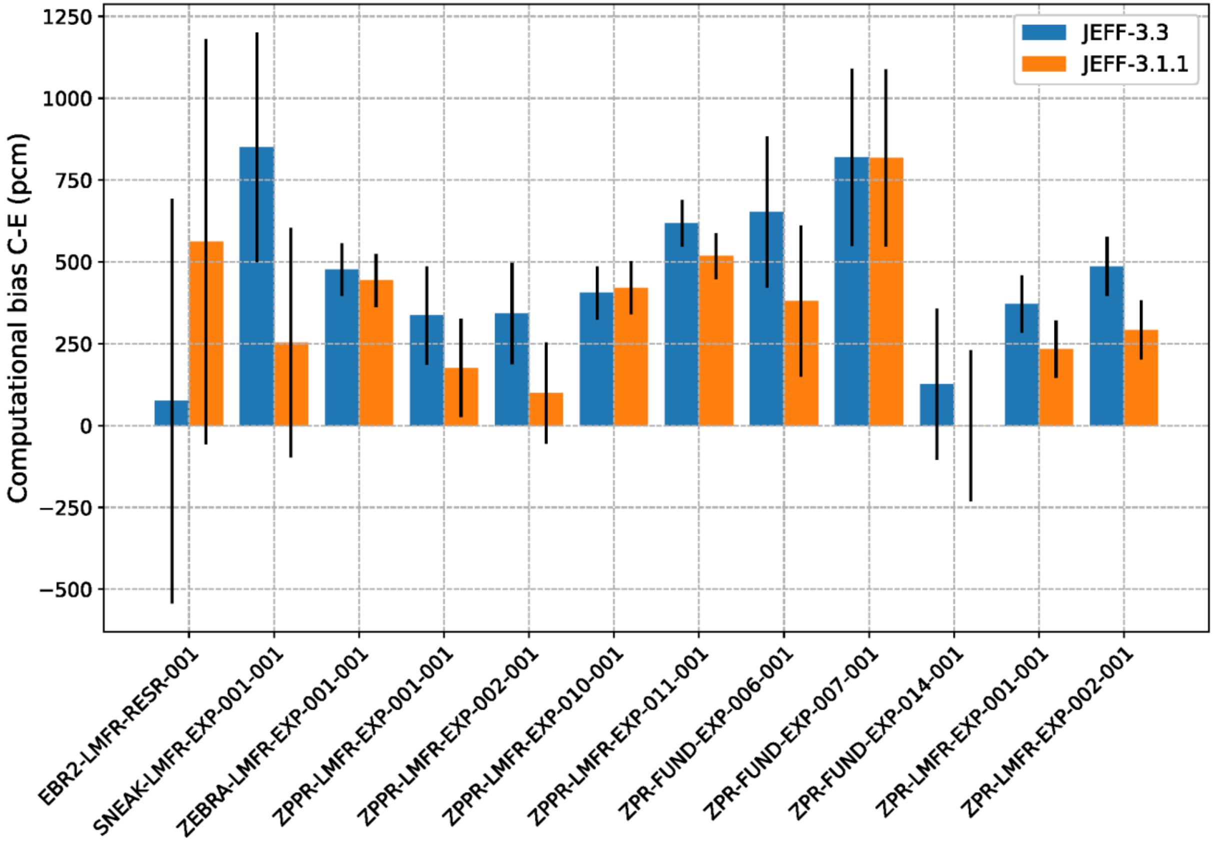
Integral experiments selection (IRPhEP)

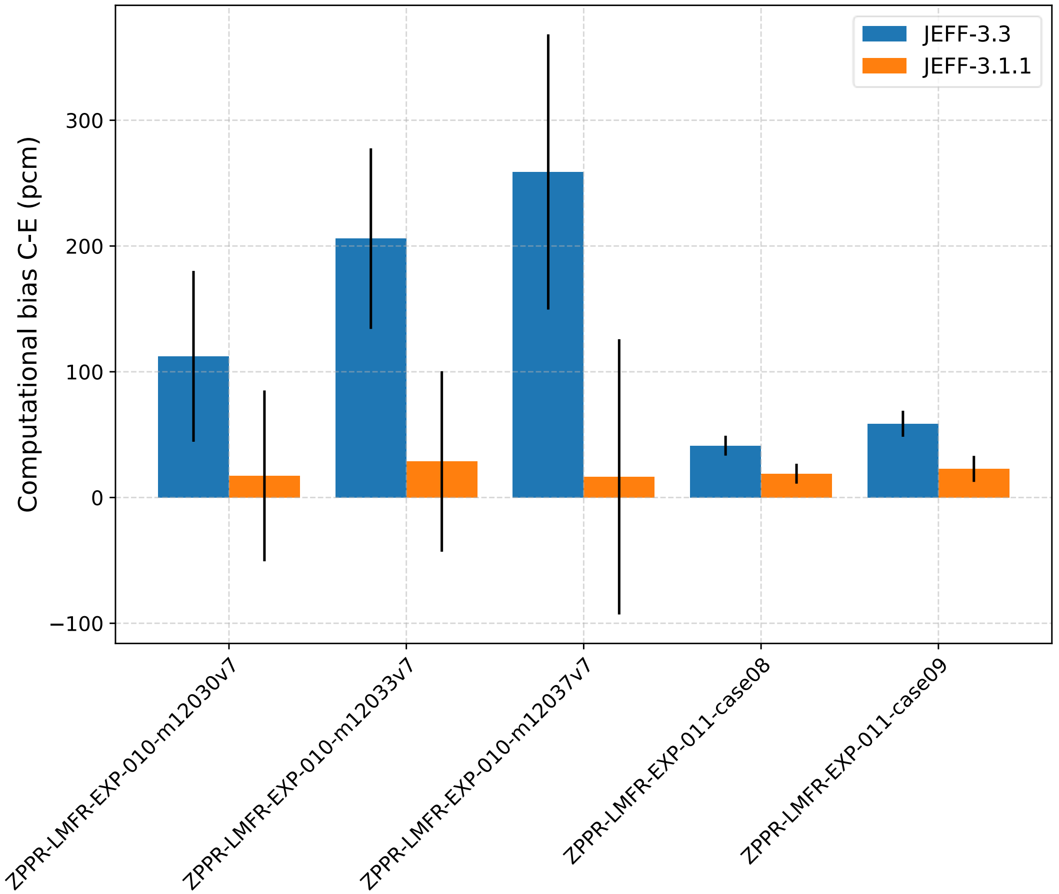
A set of **12 reactor physics experiment benchmarks from ICSBEP** is selected based on the representativity factor with ESFR, with **5 sodium void reactivity cases associated** as well as experiments dedicated to Doppler effect and Control Rod Worth analysis (SEFOR, FFTF).





Results for integral experiments (C/E)





Data assimilation for IRPhEP data set

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Impact of data assimilation on SFR designs parameters

Reactor	Response	Prior value	Posterior value	Bias (pcm)	Prior uncertainty (%)	Posterior uncertainty (%)
ESFR	Multiplication factor k_{eff}	1.00378	1.00130	-250	1.036	0.306
	Sodium void effect ρ_{Na}	500	450	**-50**	15.68	7.71
	Doppler effect ρ_T	-134	-136	-2	4.41	2.56
ASTRID	Multiplication factor k_{eff}	1.00296	1.00040	-260	0.970	0.249
	Sodium void effect ρ_{Na}	-375	-443	**-68**	22.55	10.02

- Results are now consistent with derived trends associated to representative experiments.
- k_{eff} results are mostly improve due to U-239 (n,n'), (n,f) and (n,γ) and Pu-239 $\bar{\nu}$ adjustments.
- ρ_{Na} values mostly improve due to Pu-239 (n,f) and Fe-56 (n,n) changes.

A. Jiménez-Carrascosa. "Methodologies for enhancing the neutronic assessment of Sodium-cooled Fast Reactors: from nuclear data to transient analysis," **PhD Thesis**, UPM, 2023.

Conclusions and future work

Main outcomes of the analysis

- Framework for nuclear data validation targeting SFR analyses: recommendations on related ND needs
- Role of integral experiments on the nuclear data life cycle in combination with data assimilation techniques
- This framework allows to evaluate the nuclear data performance for SFR analyses, providing recommendations on related needs and priorities.
- TSURFER as a key computational tool.

Future work

- SCALE/SAMPLER methodology for assessing correlation in experiment uncertainties.
- Extension of SCALE capabilities to include kinetic parameters.
- Comprehensive experimental database for extended adjustment analyses.
- SCALE is being applied for the assessment of the latest JEFF-4T2 library.

Acknowledgments

This work is part of the SANDA project (Supplying Accurate Nuclear Data for energy and non-energy Applications) that has received funding from the European Union’s H2020/Euratom under grant agreement No. 847552